2,2-Dimethylpropane-1,3-diol

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 7.06

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 5.62e-01

Nearest Neighbors from the Training Set

Image not found
Salicylic acid
Measured: 7.44
Predicted: 7.60

Image not found
4-Hydroxybenzoic acid
Measured: 8.08
Predicted: 7.78

Image not found
1-Hexanol
Measured: 5.18
Predicted: 4.67

Image not found
Cyclohexanol
Measured: 5.18
Predicted: 4.72

Image not found
Dipropylamine
Measured: 3.59
Predicted: 4.37